FINITE ELEMENT BASED FORMULATION OF THE LATTICE BOLTZMANN EQUATION

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Received September 8, 2008
Accepted for Publication November 24, 2008

The finite element based lattice Boltzmann method (FELBM) has been developed to model complex fluid domain shapes, which is essential for studying fluid-structure interaction problems in commercial nuclear power systems, for example. The present study addresses a new finite element formulation of the lattice Boltzmann equation using a general weighted residual technique. Among the weighted residual formulations, the collocation method, Galerkin method, and method of moments are used for finite element based Lattice Boltzmann solutions. Different finite element geometries, such as triangular, quadrilateral, and general six-sided solids, were used in this work. Some examples using the FELBM are studied. The results were compared with both analytical and computational fluid dynamics solutions.

KEYWORDS : Fluid-structure Interaction, Finite Element Method, Lattice Boltzmann Method, Three-dimensional Analysis

1. INTRODUCTION

The Lattice Boltzmann Method (LBM) has been developed for applications involving thermal-fluid problems. It is particularly attractive because of its simplicity and substantial potential for use in massively parallel computing environments compared to other currently available numerical methods. In addition, incorporation of irregular boundary conditions, mesoscopic forces that drive phase transitions, and other related complexities which are hard to be described in continuum approaches are relatively simple in the LBM formalism [1]. Recently, the technique was also applied to model fluid-structure interaction problems [2]. Most of those studies considered regular lattices, such as square and cubic grids. In order to apply the LBM to more practical cases, however, one must consider complex and irregularly shaped problem domains. Different approaches have addressed this concern. The most common technique uses the finite volume formulation of the LBM [3,4]. Other approaches use point-wise interpolation for irregular grids [5] and finite element methods [6,7].

In generally, the finite element method is very powerful for solving fluid flow in two- and three-dimensional complex and irregular domain shapes. Here, an isoparametric element formulation is often used. It is based on a mathematical mapping of regular element shapes in the imaginary domain to more general and irregular element shapes in the physical domain [8]. Other choices of finite elements are also possible: triangular and quadrilateral shapes in 2-D, and tetrahedral, triangular prism, and general six-sided solids in 3-D. This flexibility has prompted us to implement a new finite element based formulation of the lattice Boltzmann equation using the general weighted residual technique. Among the weighted residual formulations, the collocation method, Galerkin method, and method of moments are used to develop the finite element based LBM.

The numerical stability, accuracy, and efficiency of the developed FELBM are in general, not very sensitive to the choice of weighted residual method (collocation, Galerkin, and moment). Thus, in this study, for the sake of simplicity and ease, the Galerkin method implementation is selected. We develop our simulation code based on this implementation for present and future work. The *continuous* Galerkin method used in this paper is different from the *discontinuous* Galerkin method. Each technique has its merits. The former is simpler in formulation than the latter. This work differs from previous work in that a general weighted residual formulation is used for LBM solutions. This allows various FELBM to be developed, such as Galerkin's method, the collocation method, and the method of moments, etc. Each of these techniques has its own strengths in terms of the finite element formulation.

We are able, in our formulation, to take advantage of those characteristics.

2. FINITE ELEMENT BASED LATTICE BOLTZMANN METHOD

The lattice Boltzmann equation reads

$$\frac{\partial f_\alpha}{\partial t} + \vec{e}_\alpha \cdot \nabla f_\alpha = \Omega_\alpha, \quad (1)$$

where f_α is the particle velocity distribution function along the α- direction, t is time, $\vec{e}_\alpha$ is the discrete velocity vector along the α- direction, and Ω_α is the collision operator. The discrete velocity vector is given below in (2) and shown in Fig. 1 for the D2Q9-a two-dimensional square lattice model with nine discrete velocity vectors.

$$\vec{e}_\alpha = \begin{cases} (0,0) & \alpha = 0 \\ c(\cos\{(\alpha-1)\pi/2\}, \sin\{(\alpha-1)\pi/2\}) & \alpha = 1 \text{ to } 4 \\ c(\sqrt{2}\cos\{(\alpha-1)\pi/2+\pi/4\}, \sqrt{2}\sin\{(\alpha-1)\pi/2+\pi/4\}) & \alpha = 5 \text{ to } 8 \end{cases} \quad (2)$$

where c is the lattice speed.
When a single relaxation time technique is used for the collision operator, *c.f.* Bhatnagar-Gross-Krook (BGK) [9], the collision operator can be written as

$$\Omega_\alpha = -\frac{1}{\tau}\left(f_\alpha - \tilde{f}_\alpha\right), \quad (3)$$

where τ is the relaxation constant and $\tilde{f}_\alpha$ denotes the local equilibrium distribution of f_α. The latter can be derived from the Maxwell-Boltzmann distribution. Using its quadratic expansion, the local equilibrium distribution for the D2Q9 model is

$$\tilde{f}_\alpha = \rho\omega_\alpha \left[1 + \frac{3\vec{v}\cdot\vec{e}_\alpha}{c^2} + \frac{9(\vec{v}\cdot\vec{e}_\alpha)^2}{2c^4} - \frac{3\vec{v}\cdot\vec{v}}{2c^2}\right], \quad (4)$$

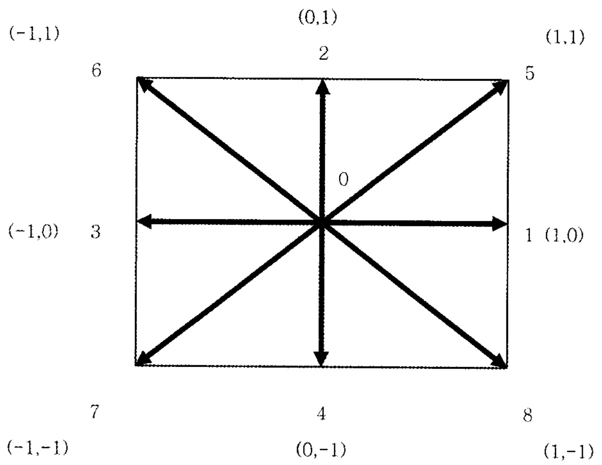

Fig. 1. D2Q9 Lattice Showing Nine Discrete Velocity Vectors

where, ρ is the fluid density and $\vec{v}$ is the fluid velocity. The fluid density ρ and momentum density $\rho\vec{v}$ are defined by sums over the particle velocity distribution function f_α, and they are expressed as

$$\rho = \sum_\alpha f_\alpha \quad (5)$$

and

$$\rho\vec{v} = \sum_\alpha f_\alpha \vec{e}_\alpha. \quad (6)$$

In addition, ω_α is the weighting parameter for each velocity direction as given below for D2Q9:

$$\omega_\alpha = \begin{pmatrix} 4/9 & \alpha = 0 \\ 1/9 & \alpha = 1,2,3,4 \\ 1/36 & \alpha = 5,6,7,8 \end{pmatrix}. \quad (7)$$

Substitution of (3) into (1) results in

$$\frac{\partial f_\alpha}{\partial t} + \vec{e}_\alpha \cdot \nabla f_\alpha + \frac{1}{\tau}\left(f_\alpha - \tilde{f}_\alpha\right) = 0. \quad (8)$$

In order to derive the FELBM from (8), the problem domain is discretized into a number of finite elements. Then, the variable f_α is expressed in terms of the interpolation functions and nodal variables as given below:

$$f_\alpha = \sum_{i=1}^{n} H^i f_\alpha^i = [H]\{f_\alpha\}, \quad (9)$$

in which H^i is the spatial interpolation function for the nodal variable f_α^i at the i-th node of the finite element, and n is the number of nodes per element. In addition, $[H]$ is a row vector consisting of the interpolation functions, and $\{f_\alpha\}$ is a column vector containing unknown solutions at the nodes. Inserting (9) into (8) yields

$$[H]\{\dot{f}_\alpha\}+\vec{e}_\alpha\cdot[\nabla H]\{f_\alpha\}+\frac{1}{\tau}[H](\{f_\alpha\}-\{\tilde{f}_\alpha\})=0 \quad (10)$$

for each finite element. The superimposed dot denotes the temporal derivative.

Applying the weighted residual formulation to (10) gives the following expression

$$\sum\int_{S_e}\{w\}\left([H]\{\dot{f}_\alpha\}+\vec{e}_\alpha\cdot[\nabla H]\{f_\alpha\}+\frac{1}{\tau}[H](\{f_\alpha\}-\{\tilde{f}_\alpha\})\right)dS=0, \quad (11)$$

where the integration is over each finite element domain S_e, and the summation is performed over the total number of elements. Furthermore, $\{w\}$ is a column vector of the weighting functions. The size of $\{w\}$ is equal to the number of nodes per element. Rewriting (11) yields

$$[M]\{\dot{F}_\alpha\}+[K]\{F_\alpha\}+[C]\{F_\alpha\}-[C]\{\tilde{F}_\alpha\}=0, \quad (12)$$

where

$$[M]=\sum[m]=\sum\int_{S_e}\{w\}[H]dS \quad (13)$$

$$[K]=\sum[k]=\sum\int_{S_e}\{w\}(\vec{e}_\alpha\cdot[\nabla H])dS \quad (14)$$

$$[C]=\sum[c]=\sum\int_{S_e}\frac{1}{\tau}\{w\}[H]dS \quad (15)$$

$$\{F_\alpha\}=\sum\{f_\alpha\} \quad (16)$$

$$\{\tilde{F}_\alpha\}=\sum\{\tilde{f}_\alpha\} \quad (17)$$

Depending on the choice of weighting function, the subsequent technique reduces to the Galerkin method, collocation method, method of moments, least-square method, or sub-domain method. In this study, the first three techniques will be investigated and implemented.

For the Galerkin method, the weighting function is selected to be the interpolation functions as used in (11), i.e. $\{w\}=[H]^T$. In this case, (13) through (15) can be expressed as

$$[M]=\sum[m]=\sum\int_{S_e}[H]^T[H]dS \quad (18)$$

$$[K]=\sum[k]=\sum\int_{S_e}[H]^T(\vec{e}_\alpha\cdot[\nabla H])dS \quad (19)$$

$$[C]=\sum[c]=\sum\int_{S_e}\frac{1}{\tau}[H]^T[H]dS \quad (20)$$

For the collocation method, the weighting functions are selected to be Dirac delta functions. In the present formulation, Dirac delta functions are defined at the nodal points of each element. Therefore, for the 2-D case, $w(x,y)=\delta(x-x_i)\delta(y-y_j)$, where x_i and y_j are the nodal coordinate values. On the other hand, for the method of moment the weighting functions are chosen to be monomial terms such as x^py^q (where p, q are non-negative integers) starting from the lowest order.

Once the matrix equation of the first order time derivative, as given by (12), is developed from the weighted residual finite element formulation, the expression is integrated over time numerically. Many different numerical time integration techniques exist. They include, but are not limited to, forward differencing, backward differencing, Crank-Nicolson, Runge-Kutta, and predictor-corrector. We chose the forward difference technique because of its computational efficiency. When we diagonalize the matrix $[M]$, the forward difference technique becomes an explicit method. As a result, because of conditional stability, the overall computation is efficient even for small time integration step sizes Δt. If an unconditionally stable method is preferred, the Crank-Nicolson technique can be used.

The forward differencing formulation of (12) is

$$\{F_\alpha\}^{t+\Delta t}=\{F_\alpha\}^t+\Delta t[M]^{-1}\left([C]\{\tilde{F}_\alpha\}^t-[C]\{F_\alpha\}^t-[K]\{F_\alpha\}^t\right), \quad (21)$$

and it is solved given some initial and boundary conditions.

3. NUMRICAL RESULTS

We performed numerical calculations for four different examples to demonstrate the performance of our FELBM technique. We first examined two-dimensional steady-

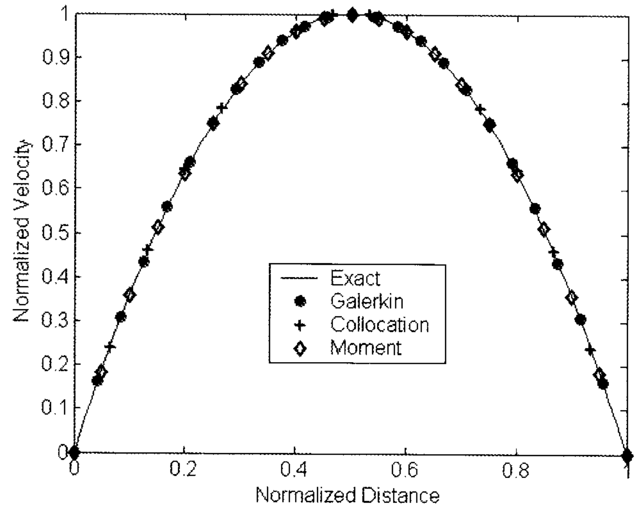

Fig. 2. Comparison of Different FELBMs (Galerkin Method, Collocation Method, and Method of Moments) for Plane Poiseuille Flow Using 2-D, Four-node Quadrilateral Elements

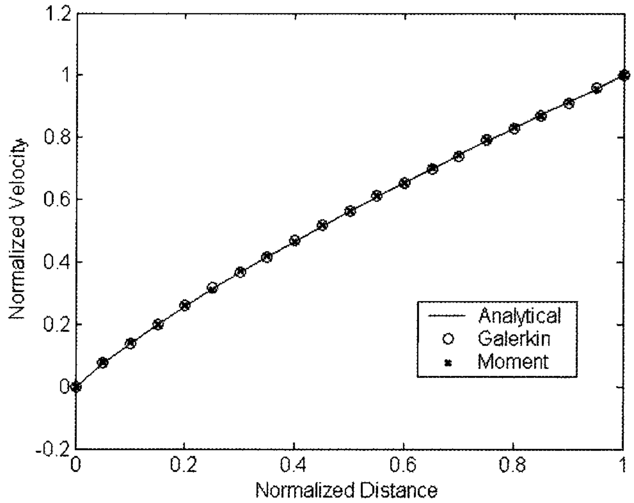

Fig. 4. Comparison of the Steady State Velocity Flow Profile between Two Co-axial Cylinders. Four-node Quadrilateral Elements were Used

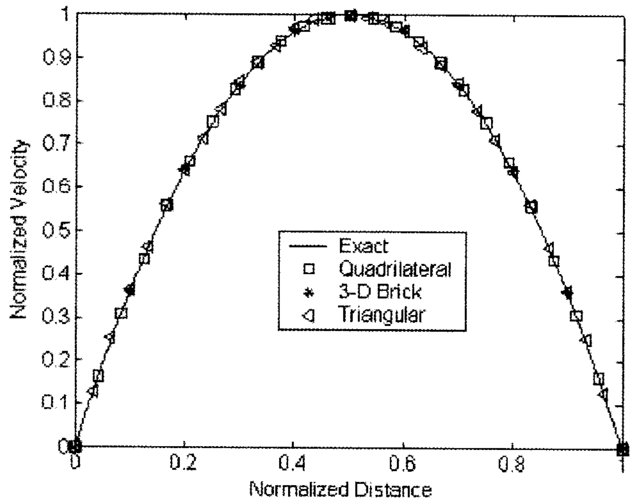

Fig. 3. Comparison of the 2-D Four-node Quadrilateral, 2-D Three-node Triangular, and 3-D Eight-node Brick-shape Elements for the Plane Poiseuille Flow Using the Galerkin Method

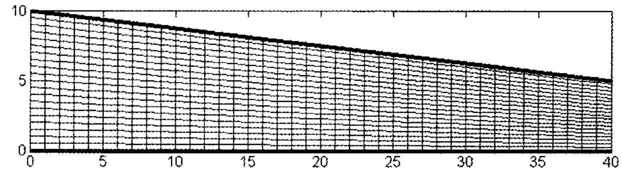

Fig. 5. Converging Duct Mesh

state Poiseuille flow between two parallel walls, where pressure was prescribed for both the duct inlet and outlet. The inlet pressure was greater than the outlet pressure, and flow occurs due to this pressure gradient since a higher pressure means greater particle velocity distribution. This problem was solved using a variety of techniques. First, the FELBM technique separately using the Galerkin, collocation, and moments methods, was applied using four-node quadrilateral elements. The finite element meshes used for the analysis ranged from 15×15 to 25×25. Their velocity profiles (Fig. 2) are in good agreement with the analytical solution. In this as well as subsequent figures, unless otherwise mentioned, all velocities were normalized with respect to the maximum velocity. The wall-spacing distance was also normalized. To avoid congestion, separate figures were plotted for each comparison. Next, we again investigated Poiseuille flow, but this time for different types of finite elements, such as three-node triangular, four-node quadrilateral, and eight-node three-dimensional solid, using the Galerkin method (Fig. 3). All solutions were in good agreement with the analytical solution.

In the second example, we investigated flow between two co-axial circular cylinders. The ratio of the radii between the outer and inner cylinders was 3. The inner cylinder was kept at rest, while the outer cylinder was rotating at a constant angular speed. The fixed velocity condition was implemented using the *bounce-back* technique for the particle velocity distribution functions so that the velocity vector from (6) becomes zero. On the other hand, for the non-zero velocity condition, the particle velocity distribution functions are properly selected to

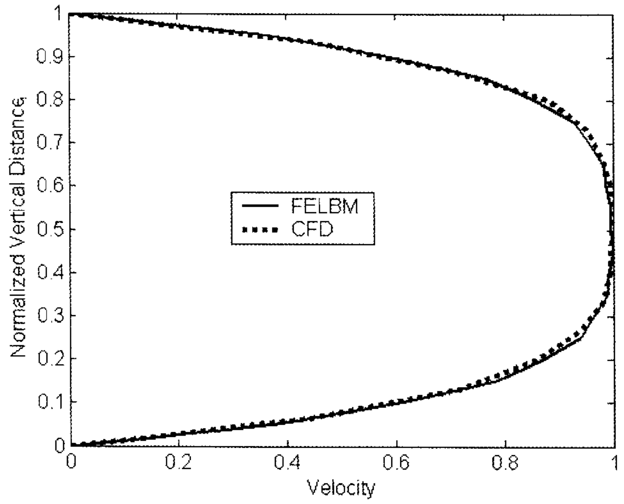

Fig. 6. Fluid Velocity at the Center of the Duct for the FELBM and CFD Methods

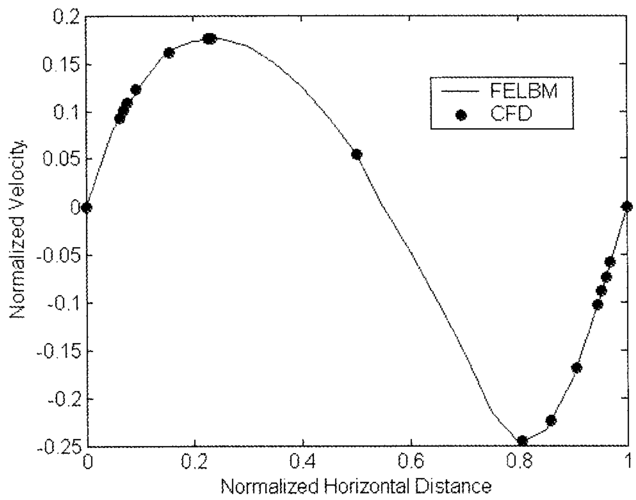

Fig. 8. Vertical Velocity Profile along the Horizontal Centerline of the Domain

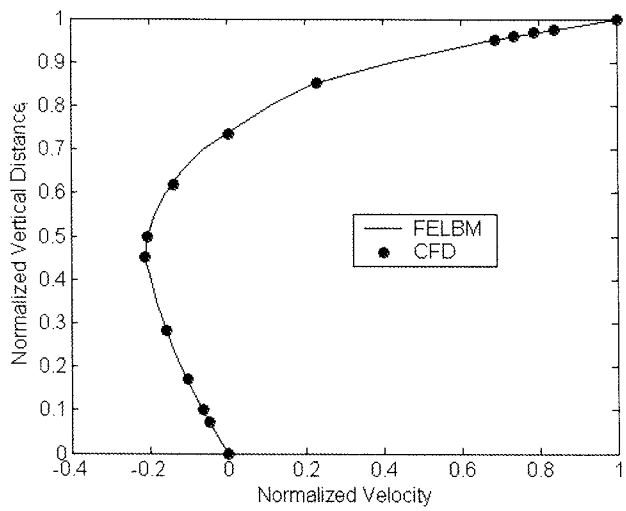

Fig. 7. Horizontal Velocity Profile along the Vertical Centerline of the Domain

satisfy the given velocity condition. The FELBM and analytical solutions are plotted in Fig. 4. Velocity in that figure is normalized with respect to the outer cylinder velocity. In addition, the inner cylinder is at zero, and the outer cylinder is at one. Both the Galerkin method and the method of moment were used with four-node quadrilateral finite elements. The numerical results are in good agreement with the exact solution.

In the third example, we investigated flow in a linearly converging duct. Its geometry and mesh is shown in Fig. 5. A pressure difference was applied between the left inlet and right outlet. Density was determined from pressure using the pressure-density relation. The inlet and outlet particle velocity distribution functions were computed for the given density and they were then prescribed along the boundaries. Transient flow analyses were conducted using FELBM and traditional CFD employing the finite volume method. After 10,000 time steps, the two solutions were compared in Fig. 6, and they are in good agreement.

In the final example, we investigated cavity driven flow. The top side of the cavity was given contact velocity u. The other sides were rigid walls. The Reynolds number ud/ν was considered to be 100, where d is the dimension of the square cavity, and ν is the fluid kinematical viscosity. The present FELBM solution was obtained using a 20×20 mesh with four-node quadrilateral elements. The results were compared to the CFD solution from Ref. [10]. Fig. 7 shows the horizontal velocity profile along the vertical centerline of the domain, while Fig. 8 shows the vertical velocity across the horizontal centerline of the domain. There is good agreement between the two solutions for both velocities.

4. CONCLUSIONS

A lattice Boltzmann technique based on the weighted residual finite element formulation was developed. This technique is able to simulate complex domain shapes essential for fluid-structure interaction studies in commercial nuclear power systems.

Four different numerical examples were presented to demonstrate the developed FELBM technique. The first example investigated two-dimensional steady-state Poiseuille flow between two parallel walls. The FELBM techniques using the Galerkin, collocation, and moments methods all using four-node quadrilateral elements were applied to the problem. Additional element geometries were used for the Galerkin method. All solutions agreed well with the analytical solution. The second example investigated flow between two co-axial circular cylinders. Both the Galerkin method and the method of moment used four-node quadrilateral finite elements. The numerical results are in good agreement with the exact solution. The third example investigated flow in a linearly converging duct. Transient flow analyses were conducted using FELBM and traditional CFD. It was shown that the two solutions are in good agreement. The last example investigated cavity driven flow. The FELBM and CFD solutions were compared. The horizontal and vertical velocity profiles as calculated by both FELBM and CFD are in good agreement.

Our results indicated that FELBM, as developed in this work, is a promising method that can be used for the study of fluid-structure interaction problems.

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